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THE SPECTRUM OF THE FORCE-BASED QUASICONTINUUM OPERATOR FOR A HOMOGENEOUS PERIODIC CHAIN*

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Abstract. We show under general conditions that the linearized force-based quasicontinuum (QCF) operator has a real, positive spectrum. The spectrum is identical to that of the quasinonlocal quasicontinuum (QNL) operator in the case of second-neighbor interactions. We construct an eigenbasis for the linearized QCF operator whose condition number is uniform in the number of atoms and the size of the atomistic region. These results establish the validity of and improve upon recent numerical observations [M. Dobson, M. Luskin, and C. Ortner, *Comput. Methods Appl. Mech. Engrg.*, 200 (2011), pp. 2697–2709, *Multiscale Model. Simul.*, 8 (2010), pp. 782–802]. As immediate consequences of our results we obtain rigorous estimates for convergence rates of (preconditioned) GMRES algorithms as well as a new stability estimate for the QCF method.

Key words. force-based atomistic/continuum coupling, stability, spectrum

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1. Introduction.

Quasicontinuum methods are a prototypical class of multiscale methods that directly couple multiple modeling regions to reduce the computational complexity of modeling large atomistic systems. These methods are useful for computing the interaction of localized material defects such as crack tips or dislocations with long-range elastic fields of a crystalline material. The force-based quasicontinuum (QCF) method [3, 4, 21] partitions the material into two disjoint regions, the atomistic region and the continuum region. It assigns forces to the degrees of freedom within each region using only the respective model, be it atomistic or continuum. This simplifies the formulation of the method, as no special interaction rules are needed near the atomistic/continuum interface. The simplicity of mixing forces combined with the lack of spurious interface forces (so-called ghost forces) makes the force-based coupling method a widely applied concept in the multiscale literature [1, 2, 3, 12, 14, 21, 22].

A potential drawback of the QCF method is that it does not derive from an energy (as it generally produces a nonconservative field). In particular, this implies that the linearized QCF operator, which we denote by L^{qcf}, is not symmetric. While the practical implications of this fact are still under investigation, it is already clear that the analysis of the QCF method poses formidable challenges. A series of recent articles has been devoted to its study [8, 6, 7]. These works are restricted to one dimension

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and typically consider the case of a linearized operator with first- and second-neighbor interactions only. For example, if we let N denote the number of atoms in the chain, it was shown in [6, 7] that, for N sufficiently large, L^{qcf} is *not* positive definite. (We emphasize that a nonsymmetric, indefinite operator may nevertheless have a positive spectrum of eigenvalues; that is, our new results do not contradict the lack of positivity of L^{qcf}.) It was, moreover, shown that L^{qcf} is not uniformly stable in N in discrete variants of most Sobolev spaces.

However, numerical experiments in [8, 6] showed some unexpected spectral properties. Conjecture 2 in [6] states that the spectrum of ℓ^2-eigenvalues of the second-neighbor linearized QCF operator is identical to that of the operator associated with the quasinonlocal quasicontinuum (QNL) method [23]. This is particularly surprising since the QNL method is energy based, and thus indicates that the linearized QCF operator is diagonalizable and that its spectrum is real. Furthermore, Conjecture 8 in [8] states that the condition number of a matrix of eigenvectors of the QCF operator grows at most logarithmically.

The purpose of the present paper is to provide rigorous proofs for these numerical observations and to extend the results to the case of finite-range interactions. We define the QCF method and introduce the necessary notation in section 2. In section 3 we establish all results in the case of second-neighbor interactions as in the numerical experiments in [8, 6]. Then, in section 4 we extend the results to the more technical case of finite-range interactions. The fact that the spectrum for the linearized QCF operator is identical to that of the QNL operator is specific to the second-neighbor case, not only since there is no single generalization of QNL but also because a general similarity relation is impossible as discussed in Remark 4.3. We instead examine when the spectrum is real and positive. In the case of finite-range interactions we give sufficient conditions for the existence of a real positive spectrum and prove an estimate on the eigenvalues of L^{qcf} in terms of the eigenvalues of the atomistic and continuum operators, which are easily characterized (Theorem 4.7).

We note, moreover, that we were able to construct a matrix of eigenvectors for the linearized QCF operator whose condition number is bounded uniformly in the number of atoms and the size of the atomistic region. This result is in fact stronger than the conclusions made in [8] from numerical observations (we used a different scaling of the eigenbasis). Our new estimates are used in section 5.1 to give bounds on the convergence rate of standard and preconditioned GMRES iterations. Finally, in section 5.2 we prove a new sharp stability estimate for the linearized QCF operator.

2. Formulation of the QCF method. For the sake of brevity, we will keep the introduction to the atomistic model and the various flavors of quasicontinuum approximations to a minimum. We refer the reader to [4, 8, 6, 7, 10, 15, 16, 17] for detailed discussions. Note, in particular, that we have left out the usual rescaling factor ε. This reduces the complexity of the notation and is justified since in this paper we are primarily concerned with algebraic aspects of quasicontinuum operators.

2.1. Notation for difference operators. In this section, we summarize the notation and certain elementary results for some standard finite difference operators with periodic boundary conditions.

2.1.1. Periodic domains. We identify $\mathbb{R}^N$ with periodic infinite sequences as follows:

$$\mathbb{R}^N = \big\{u \in \mathbb{R}^{\mathbb{Z}} : u_{\ell+N} = u_\ell \ \forall \ell \in \mathbb{Z}\big\}.$$

The ℓ^2–inner product on $\mathbb{R}^N$ and its associated norm are defined by

$$\langle u, v\rangle = u^T v = \sum_{\ell=1}^{N} u_\ell v_\ell \quad \text{and} \quad \|u\| = \sqrt{\langle u, u\rangle}.$$

We will frequently use a subspace $\mathcal{U} \subset \mathbb{R}^N$ of mean zero functions,

$$\mathcal{U} = \big\{u \in \mathbb{R}^N : \langle u, e\rangle = 0\big\}, \tag{2.1}$$

where $e = (1)_{\ell\in\mathbb{Z}} \in \mathbb{R}^N$.

The orthogonal projection onto $\mathcal{U}$ is denoted by $P_{\mathcal{U}} : \mathbb{R}^N \to \mathbb{R}^N$,

$$(P_{\mathcal{U}} u)_\ell = u_\ell - \frac{1}{N}\sum_{k=1}^{N} u_k,$$

or, in matrix notation,

$$P_{\mathcal{U}} = I - \tfrac{1}{N} e \otimes e. \tag{2.2}$$

2.1.2. The backward difference operator. The difference operator $D : \mathbb{R}^N \to \mathbb{R}^N$ is defined by

$$Du_\ell = (Du)_\ell = u_\ell - u_{\ell-1}.$$

We note that $\mathrm{rg}(D) = \mathcal{U}$ and $\ker(D) = \mathrm{span}\{e\}$, where rg denotes the range and ker denotes the kernel of an operator. We also remark that, here and throughout, unless specifically stated otherwise, we will not distinguish between an operator and its associated matrix representation in $\mathbb{R}^{N\times N}$.

2.1.3. The discrete Laplace operator. The second generic operator that we will encounter is the negative Laplace operator $L : \mathbb{R}^N \to \mathbb{R}^N$,

$$Lu_\ell = (Lu)_\ell = -u_{\ell-1} + 2u_\ell - u_{\ell+1}.$$

As for the difference operator, $\mathrm{rg}(L) = \mathcal{U}$ and $\ker(L) = \mathrm{span}\{e\}$.

Using summation by parts, we obtain

$$\langle Lu, v\rangle = \langle Du, Dv\rangle,$$

which implies that $L = D^T D$ and hence $L = L^T$. Since $Le = 0$, we have the identities

$$LP_{\mathcal{U}} = P_{\mathcal{U}} L = L. \tag{2.3}$$

We also note that $\|L\| \le 4$, and that this bound is attained for even N, as well as in the limit $N \to \infty$.

Since L is singular, we also define the modified negative Laplace operator

$$L_1 = L + e \otimes e = L + (I - P_{\mathcal{U}}), \tag{2.4}$$

so that $L_1 u = Lu$ if $u \in \mathcal{U}$ and $L_1 e = e$. This operator is invertible and satisfies

$$L_1^{-1} L = L L_1^{-1} = P_{\mathcal{U}}.$$

2.1.4. The translation operator. The translation operator $T : \mathbb{R}^N \to \mathbb{R}^N$ is defined by

$$Tu_\ell = (Tu)_\ell = u_{\ell+1}. \tag{2.5}$$

T is an orthogonal operator, i.e., $T^T T = I$, and its eigenbasis can be written explicitly as

$$Tw_k = \lambda_k w_k, \quad \lambda_k = e^{\frac{i2\pi k}{N}}, \quad (w_k)_\ell = e^{\frac{i2\pi k\ell}{N}} \quad \text{for } 1 \le k \le N. \tag{2.6}$$

The eigenvalues of T are located on the unit circle $\mathcal{T} := \{t \in \mathbb{C} : \ |t| = 1\}$ and, in the limit $N \to \infty$, are dense in $\mathcal{T}$.

We remark that we can write the difference operator D and the negative Laplace operator as Laurent polynomials in T: $D = p_D(T)$ and $L = p_L(t)$, where

$$p_D(t) = (1 - t^{-1}) \quad \text{and} \quad p_L(t) = (-t + 2 - t^{-1}).$$

In general, if $p(t)$ is a polynomial, then the spectrum of the operator $p(T)$ is $\{p(\lambda_k) : 1 \le k \le N\}$, and the eigenvectors are the same as for T. Since T is a normal operator, all polynomials $p(T)$ are also normal.

Finally, we note that $Te = e$, which implies that T or any polynomial of T commutes with $e \otimes e$. In particular, this implies that all polynomials in T (e.g., L, D) and the operators L_1 and $P_{\mathcal{U}}$ commute.

2.2. The linearized atomistic operators. We consider an atomistic model problem with periodic boundary conditions. We let $\mathcal{U}$ be the set of admissible displacements of an N-periodic chain: the set of all N-periodic displacements with mean zero. The latter condition is necessary to ensure that the systems of equations that we consider are well posed. If $F > 0$ is a fixed *macroscopic strain*, then the energy (per period) of the atomistic chain subject to a displacement $u \in \mathbb{R}^N$ is given by

$$\mathcal{E}^{\mathrm{a}}(u) = \sum_{r=1}^{R} \sum_{\ell=1}^{N} \phi\big(rF + (u_\ell - u_{\ell-r})\big),$$

where $\phi \in \mathrm{C}^2(0, +\infty)$ is a pair interaction potential, for example, a Lennard-Jones or Morse potential, and $R \in \mathbb{N}$, $R \ge 2$, can be thought of as a discrete cutoff radius. (Note that, even though we have defined $\mathcal{E}^{\mathrm{a}}$ for all $u \in \mathbb{R}^N$, only $u \in \mathcal{U}$ are admitted in the solution of the minimization problem.)

The Cauchy–Born or local quasicontinuum (QCL) approximation of $\mathcal{E}^{\mathrm{a}}$ is the functional

$$\mathcal{E}^{\mathrm{c}}(u) = \sum_{\ell=1}^{N} W\big(F + (u_\ell - u_{\ell-1})\big) = \sum_{\ell=1}^{N} W\big(F + Du_\ell\big),$$

where W is the *Cauchy–Born stored energy function*, $W(s) = \sum_{r=1}^{R} \phi(rs)$.

Our analysis in the present paper concerns properties of the Hessians

$$[L^{\mathrm{a}}_{ij}] = \left[\frac{\partial^2 \mathcal{E}^{\mathrm{a}}}{\partial u_i \partial u_j}\right]\Big|_{u=0}, \qquad [L^{\mathrm{c}}_{ij}] = \left[\frac{\partial^2 \mathcal{E}^{\mathrm{c}}}{\partial u_i \partial u_j}\right]\Big|_{u=0} \tag{2.7}$$

and the quasicontinuum operators that we derive from them. For future reference we write out L^{a} and L^{c} explicitly:

$$(L^{\mathrm{a}}u)_\ell = \sum_{r=1}^{R} \phi''_{rF}(-u_{\ell+r} + 2u_\ell - u_{\ell-r}) \tag{2.8}$$

and

$$(L^{\mathrm{c}}u)_\ell = \sum_{r=1}^{R} \phi''_{rF} r^2(-u_{\ell+1} + 2u_\ell - u_{\ell-1}) = W''_F\ (Lu)_\ell, \tag{2.9}$$

where the constants ϕ''_{rF} and W''_F are given by

$$\phi''_{rF} = \phi''(rF) \quad \text{and} \quad W''_F = W''(F) = \sum_{r=1}^{R} \phi''_{rF} r^2.$$

We have written both L^{a} and L^{c} as linear operators from $\mathbb{R}^N$ to $\mathbb{R}^N$, but both map $\mathcal{U}$ to $\mathcal{U}$. As maps from $\mathbb{R}^N$ to $\mathbb{R}^N$ both operators have a nontrivial kernel that contains e, but we are primarily interested in their properties on $\mathcal{U}$. For example, we note that if $\phi''_F > 0$, $\phi''_{rF} \le 0$ for $r \ge 2$ and $W''_F > 0$, then both are positive definite on $\mathcal{U}$ and, in particular, invertible (see [6, eq. (2.2) and sect. 2.2] and [5, Props. 1 and 2] for the second-neighbor case and [11] for finite range). For the continuum operator, L^{c}, the stability condition $W''_F > 0$ is sharp; that is, L^{c} is positive definite if and only if $W''_F > 0$. We work to prove our spectral results on the quasicontinuum operators up to this sharp stability criterion on the coefficients.

2.3. The force-based quasicontinuum method. The force-based quasicontinuum (QCF) method is obtained by mixing the forces from the atomistic and the continuum models. To this end, we define atomistic and continuum regions $\mathcal{A}$ and $\mathcal{C}$ that satisfy

$$\mathcal{A} \cup \mathcal{C} = \{1, \dots, N\} \quad \text{and} \quad \mathcal{A} \cap \mathcal{C} = \emptyset. \tag{2.10}$$

We define the QCF forces

$$F_\ell^{\mathrm{qcf}}(u) = \begin{cases} -\frac{\partial \mathcal{E}^{\mathrm{a}}(u)}{\partial u_\ell} & \text{if } \ell \in \mathcal{A}, \\ -\frac{\partial \mathcal{E}^{\mathrm{c}}(u)}{\partial u_\ell} & \text{if } \ell \in \mathcal{C}. \end{cases}$$

Linearization of the nonlinear QCF operator $F(u) = (F_\ell^{\mathrm{qcf}}(u))_{\ell=1}^N$ at $u = 0$ yields the *linearized QCF operator* (or simply, *QCF operator*), $L^{\mathrm{qcf}} : \mathbb{R}^N \to \mathbb{R}^N$,

$$(L^{\mathrm{qcf}}u)_\ell = \begin{cases} (L^{\mathrm{a}}u)_\ell & \text{if } \ell \in \mathcal{A}, \\ (L^{\mathrm{c}}u)_\ell & \text{if } \ell \in \mathcal{C}, \end{cases} \tag{2.11}$$

which is the focus of our studies in the present paper.

Unfortunately, L^{qcf} as defined above does not map $\mathcal{U}$ to $\mathcal{U}$; hence we will normally consider the projected QCF operator (see [6, sect. 2.3] for more details)

$$L_0^{\mathrm{qcf}} = P_{\mathcal{U}} L^{\mathrm{qcf}}.$$

To conclude this section we represent L^{qcf} in a more compact way. By considering the characteristic function of $\mathcal{A}$,

$$\chi_\ell = \begin{cases} 1 & \text{if } \ell \in \mathcal{A}, \\ 0 & \text{if } \ell \in \mathcal{C}, \end{cases}$$

and the associated diagonal operator $X : \mathbb{R}^N \to \mathbb{R}^N$,

$$(Xu)_\ell = \chi_\ell u_\ell,$$

we can write L^{qcf} in the form

$$L^{\mathrm{qcf}} = [1 - X]L^{\mathrm{c}} + XL^{\mathrm{a}} = L^{\mathrm{c}} + X[L^{\mathrm{a}} - L^{\mathrm{c}}]. \tag{2.12}$$

2.4. The quasinonlocal quasicontinuum method. The second atomistic/continuum hybrid scheme that will feature prominently in our investigations is the *quasinonlocal quasicontinuum (QNL) method* [23]. We note that the QNL method is defined only for second-neighbor interaction range (i.e., $R = 2$). Extensions to further neighbors exist [10, 13, 20], but we use only the version up to second neighbors in this paper. The QNL method is conservative with energy functional

$$\begin{aligned} \mathcal{E}^{\mathrm{qnl}}(u) = & \sum_{\ell \in \mathcal{A} \cup \mathcal{C}} \phi\big(F + (u_\ell - u_{\ell-1})\big) + \sum_{\ell \in \mathcal{A}} \phi\big(2F + (u_{\ell+1} - u_{\ell-1})\big) \\ & + \sum_{\ell \in \mathcal{C}} \frac{1}{2}\Big\{\phi\big(2F + 2(u_\ell - u_{\ell-1})\big) + \phi\big(2F + 2(u_{\ell+1} - u_\ell)\big)\Big\}. \end{aligned}$$

The linearized QNL operator $L^{\mathrm{qnl}} : \mathbb{R}^N \to \mathbb{R}^N$ is the Hessian of $\mathcal{E}^{\mathrm{qnl}}$ at $u = 0$. It is most naturally written in variational form [5, sect. 4.3] as

$$\langle L^{\mathrm{qnl}} u, v\rangle = W_F'' \sum_{\ell \in \mathcal{A} \cup \mathcal{C}} Du_\ell Dv_\ell - \phi_{2F}'' \sum_{\ell \in \mathcal{A}} Lu_\ell Lv_\ell. \tag{2.13}$$

Based on this representation one can show that if $W_F'' > 0$ and $\phi_F'' > 0$, then L^{qnl} is positive definite on $\mathcal{U}$. (For $\phi_{2F}'' \le 0$ this follows from (2.13); for $\phi_{2F}'' > 0$ it follows from the basic representation $\langle L^{\mathrm{qnl}} u, u\rangle = \phi_F''\langle Du, Du\rangle + \phi_{2F}''\langle D_2 u, D_2 u\rangle$, where $D_2 u_\ell = u_\ell - u_{\ell-2}$.)

3. The ℓ^2-spectrum of the second-neighbor L^{qcf} operator. In [6] the invertibility of the QCF operator was investigated analytically and numerically, and various numerical observations regarding the spectrum were made. In the present section we confirm these numerical experiments by proving, in the second-neighbor case, that the QCF operator has a real spectrum, which is identical to the spectrum of the QNL operator.

In section 4, devoted to finite-range interactions, we establish that there is, in general, no energy-based quasicontinuum method whose linearized operator has a spectrum that is identical to the spectrum of the QCF operator (refer to Remark 4.3 for details). Nevertheless, we will show that the QCF operator is similar to a symmetric matrix, which allows us to extend most of our results to finite-range interactions.

The purpose of a separate analysis of the second-neighbor case serves to motivate the finite-range analysis in a technically much simpler setting and to obtain more explicit estimates for this important special situation.

3.1. Similarity of $L_0^{\rm qcf}$ and $L^{\rm qnl}$. In [8, 6] it was observed in numerical experiments that the spectra of $L_0^{\rm qcf}$ and $L^{\rm qnl}$ coincide. In this section we provide a rigorous proof by explicitly constructing a similarity transformation between $L_0^{\rm qcf}$ and $L^{\rm qnl}$. The main ideas, after which the proof will be straightforward, are the following two new representations of the $L^{\rm qcf}$ and $L^{\rm qnl}$ operators.

PROPOSITION 3.1. *Let $R = 2$; then $L^{\rm qcf}$ and $L^{\rm qnl}$ have, respectively, the representations*

$$L^{\rm qcf} = W_F'' L - \phi_{2F}'' X L^2 \tag{3.1}$$

and

$$L^{\rm qnl} = W_F'' L - \phi_{2F}'' L X L. \tag{3.2}$$

Proof. We begin by noting that, for $R = 2$, the operators $L^{\rm a}$ and $L^{\rm c}$ may be written as

$$\begin{aligned} L^{\rm a} &= \phi_F'' L + \phi_{2F}''[4L - L^2] = W_F'' L - \phi_{2F}'' L^2, \\ L^{\rm c} &= \phi_F'' L + \phi_{2F}''[4L] = W_F'' L. \end{aligned}$$

Using these formulas, the operator $L^{\rm qcf}$ (as defined in (2.11)) can be written in terms of the atomistic and the continuum operators (2.12) as

$$L^{\rm qcf} = X L^{\rm a} + [I - X] L^{\rm c} = X \left[W_F'' L - \phi_{2F}'' L^2 \right] + [I - X] \left[W_F'' L \right].$$

From this we immediately obtain (3.1).

To rewrite the QNL operator, we note that we can write (2.13) as

$$\begin{aligned} \langle L^{\rm qnl} u, v \rangle &= W_F'' \langle Du, Dv \rangle - \phi_{2F}'' \langle XLu, Lv \rangle \\ &= W_F'' \langle D^T Du, v \rangle - \phi_{2F}'' \langle LXLu, v \rangle \end{aligned}$$

for all $u, v \in \mathbb{R}^N$, and we therefore obtain (3.2). ∎

Based on (3.1) and (3.2) we will deduce the similarity of the QCF and QNL operators. Since L is not invertible, we introduce the nonsingular operator $L_1 : \mathbb{R}^N \to \mathbb{R}^N$ defined by (2.4). The following result confirms Conjecture 2 in [6].

THEOREM 3.2 (similarity of $L_0^{\rm qcf}$ and $L^{\rm qnl}$). *If $R = 2$, then the operators $L_0^{\rm qcf}$ and $L^{\rm qnl}$ are similar, with similarity transformation L_1 defined by* (2.4)*:*

$$L_0^{\rm qcf} = L_1^{-1} L^{\rm qnl} L_1.$$

In particular, the spectra of $L_0^{\rm qcf}$ and $L^{\rm qnl}$ coincide.

Proof. Using formulas (2.3), (3.1), and (3.2), a straightforward computation yields the desired identity:

$$\begin{aligned} L_1 L_0^{\rm qcf} &= L_1 P_{\mathcal{U}} L^{\rm qcf} = L L^{\rm qcf} \\ &= W_F'' L L - \phi_{2F}'' L X L^2 \\ &= [W_F'' L - \phi_{2F}'' L X L] L_1 = L^{\rm qnl} L_1. \end{aligned}$$

∎

3.2. Condition number of the ℓ^2-eigenbasis. Since L^{qnl} is self-adjoint, there exist an orthonormal matrix $V^{\mathrm{qnl}} \in \mathbb{R}^{N\times N}$ and a diagonal matrix Λ containing the eigenvalues of L^{qnl} such that

$$L^{\mathrm{qnl}} V^{\mathrm{qnl}} = V^{\mathrm{qnl}} \Lambda. \tag{3.3}$$

Note in particular that Λ also contains the zero eigenvalue. Since the operators L^{qnl} and L_0^{qcf} are similar, there also exists an invertible matrix $V^{\mathrm{qcf}} \in \mathbb{R}^{N\times N}$ such that

$$L_0^{\mathrm{qcf}} V^{\mathrm{qcf}} = V^{\mathrm{qcf}} \Lambda.$$

We recall the definition of the condition number of a matrix A,

$$\mathrm{cond}(A) = \|A\|\,\|A^{-1}\|.$$

A bound on the condition number of the matrix of eigenvalues is useful, for example, when estimating the convergence rate for the GMRES algorithm [19]. As suggested by Theorem 3.2, a possible choice for the eigenvectors is $L_1^{-1} V^{\mathrm{qnl}}$, since in that case we have

$$L_0^{\mathrm{qcf}}\, L_1^{-1} V^{\mathrm{qnl}} = L_1^{-1} L^{\mathrm{qnl}} V^{\mathrm{qnl}} = L_1^{-1} V^{\mathrm{qnl}}\, \Lambda.$$

However, $\mathrm{cond}(L_1^{-1} V^{\mathrm{qnl}}) = \mathrm{cond}(L_1^{-1}) = O(N^2)$, which is much worse than the numerical observations in [6] and suggests a poor scaling of the eigenvectors.

To produce an eigenbasis with a smaller condition number, it is important to note that the choice of eigenvectors is not unique even after fixing the ordering, as we are always free to rescale them. This turns out to be a crucial ingredient in our following construction of an eigenbasis with a uniformly bounded condition number. The following result is inspired by Figure 4.2 in [6] and Conjecture 8 in [8]. It does not precisely confirm these but establishes a closely related and in fact stronger result.

THEOREM 3.3. *Suppose that $R = 2$; then the operator $V^{\mathrm{qcf}} : \mathbb{R}^N \to \mathbb{R}^N$,*

$$V^{\mathrm{qcf}} = [W_F'' I - \phi_{2F}'' P_{\mathcal{U}} X L] V^{\mathrm{qnl}}, \tag{3.4}$$

diagonalizes L_0^{qcf}, that is, $L_0^{\mathrm{qcf}} V^{\mathrm{qcf}} = V^{\mathrm{qcf}} \Lambda$, where Λ is the diagonal matrix of eigenvalues associated with L^{qnl} (3.3). Moreover, if $W_F'' > 0$ and $\phi_F'' > 0$, then $\mathrm{cond}(V^{\mathrm{qcf}})$ is bounded above by a constant that depends on ϕ_{2F}''/W_F'' but is independent of N and $\mathcal{A}$.

REMARK 3.1. *The choice of V^{qcf} is motivated by the following calculation. Starting with the similarity result of Theorem 3.2, we derive*

$$L_0^{\mathrm{qcf}} = L_1^{-1} L^{\mathrm{qnl}} L_1 = L_1^{-1} V^{\mathrm{qnl}} \Lambda (V^{\mathrm{qnl}})^T L_1,$$

and we scale the eigenvectors by Λ, which gives

$$\begin{aligned} L_1^{-1} V^{\mathrm{qnl}} \Lambda &= L_1^{-1} V^{\mathrm{qnl}} \Lambda [V^{\mathrm{qnl}}]^T V^{\mathrm{qnl}} = L_1^{-1} L^{\mathrm{qnl}} V^{\mathrm{qnl}} \\ &= L_1^{-1} [W_F'' L - \phi_{2F}'' L X L] V^{\mathrm{qnl}} = [W_F'' P_{\mathcal{U}} - \phi_{2F}'' P_{\mathcal{U}} X L] V^{\mathrm{qnl}}. \end{aligned}$$

This is equivalent to the choice of V^{qcf} in (3.4) when restricted to $\mathcal{U}$.

Proof of Theorem 3.3. *Step* 1: *Diagonalization.* In a straightforward computation we obtain

$$\begin{aligned} L_0^{\mathrm{qcf}} V^{\mathrm{qcf}} &= \left[W_F'' L - \phi_{2F}'' P_{\mathcal{U}} X L^2\right] \left[W_F'' I - \phi_{2F}'' P_{\mathcal{U}} X L\right] V^{\mathrm{qnl}} \\ &= \left[W_F'' I - \phi_{2F}'' P_{\mathcal{U}} X L\right] \left[W_F'' L - \phi_{2F}'' L X L\right] V^{\mathrm{qnl}} \\ &= \left[W_F'' I - \phi_{2F}'' P_{\mathcal{U}} X L\right] V^{\mathrm{qnl}} \Lambda \\ &= V^{\mathrm{qcf}} \Lambda. \end{aligned}$$

Step 2: *Estimating* $\mathrm{cond}(V^{\mathrm{qcf}})$. We now assume that $W_F'' > 0$ and $\phi_F'' > 0$. To estimate $\mathrm{cond}(V^{\mathrm{qcf}})$ we can ignore the positive constant multiple W_F'' as well as the orthonormal matrix V^{qnl}; that is, we have

$$\mathrm{cond}(V^{\mathrm{qcf}}) = \mathrm{cond}(A) = \|A\|\,\|A^{-1}\|, \quad \text{where} \quad A = I - \alpha P_{\mathcal{U}} X L, \tag{3.5}$$

with constant $\alpha = \frac{\phi_{2F}''}{W_F''}$, and the convention $\|A^{-1}\| = +\infty$ if A is not invertible. We recall that in the current case of second-neighbor interactions, $W_F'' = \phi_F'' + 4\phi_{2F}''$, and we note that the condition $\phi_F'', W_F'' > 0$ implies that $\alpha < 1/4$.

Elementary estimates give the upper bound

$$\|A\| \le 1 + |\alpha|\|P_{\mathcal{U}}\|\|X\|\|L\| \le 1 + 4|\alpha|. \tag{3.6}$$

We similarly get the lower bound

$$\|Au\| \ge 1 - |\alpha|\|P_{\mathcal{U}}\|\|X\|\|L\| = 1 - 4|\alpha| \qquad \forall u \text{ s.t. } \|u\| = 1, \tag{3.7}$$

which gives an estimate for $\|A^{-1}\|$ whenever $W_F'' - 4|\phi_{2F}''| > 0$. In the following we prove a bound for $\|A^{-1}\|$ that holds whenever $W_F'' > 0$, that is, up to the sharp stability limit, which is a more involved result.

To estimate $\|A^{-1}\|$ we use the fact that (i) $\|A^{-1}\| = \|A^{-T}\|$, and (ii) if

$$\|A^T u\| \ge \gamma_0 \|u\| \qquad \forall u \in \mathbb{R}^N$$

for some constant $\gamma_0 > 0$, then A^T is invertible and $\|A^{-T}\| \le 1/\gamma_0$. In Lemma 3.4 we establish precisely this fact, assuming that $\alpha < 1/4$, with a constant γ_0 that depends only on α but not on N or $\mathcal{A}$. ∎

A generalization of the following technical lemma used in the previous proof will also be required in the finite-range interaction case. It follows from Lemma 4.6 by choosing $Z = I$.

LEMMA 3.4. *Let $\alpha < 1/4$; then there exists a constant $\gamma_0 > 0$, which depends on α but is independent of N and of $\mathcal{A}$, such that*

$$\big\|[I - \alpha P_{\mathcal{U}} X L]^T u\big\| \ge \gamma_0 \|u\| \qquad \forall u \in \mathbb{R}^N.$$

REMARK 3.2. *From the proof of Lemma* 4.6 *we can derive that, in the case $\phi_{2F}'' \le 0$, the constant γ_0 is explicitly given by*

$$\gamma_0^2 = 1 + 8\alpha^2 - 4\sqrt{\alpha^2 + 4\alpha^4}, \tag{3.8}$$

where $\alpha = \phi_F''/W_F''$, and the resulting condition number estimate by

$$\mathrm{cond}(V^{\mathrm{qcf}})^2 \le \frac{(1 + 4|\alpha|)^2}{1 + 8\alpha^2 - 4\sqrt{\alpha^2 + 4\alpha^4}} =: c(\alpha)^2.$$

If ϕ_{2F}'' is moderate but $W_F'' \to 0$, then $\alpha \to -\infty$. A brief calculation shows that in this limit $c(\alpha)$ behaves asymptotically like

$$c(\alpha) \sim 2^{5/2}\alpha^2 + O(|\alpha|^{3/2}) \qquad \text{as} \quad \alpha \to -\infty.$$

4. Finite-range interactions. We recall from (2.12) the definition of the finite-range QCF operators,

$$L^{\mathrm{qcf}} = L^{\mathrm{c}} + X[L^{\mathrm{a}} - L^{\mathrm{c}}] \quad \text{and} \quad L_0^{\mathrm{qcf}} = L^{\mathrm{c}} + P_{\mathcal{U}} X[L^{\mathrm{a}} - L^{\mathrm{c}}],$$

where L^{a} and L^{c} are, respectively, the atomistic and the continuum operators defined in (2.8) and (2.9). The case $R = 2$, considered in the previous section, relied on the fact that $L^{\mathrm{a}} - L^{\mathrm{c}} = -\phi''_{2F} L^2$ is either positive or negative definite and, up to a constant, is a square of L. This allowed us to symmetrize the expression $X[L^{\mathrm{a}} - L^{\mathrm{c}}] = L^{-1}\left(-\phi''_{2F} LXL\right) L$. The fact that it was similar to a well-known quasicontinuum energy is particular to that case; for longer-range interactions the QCF operator does not have a real spectrum for all parameter choices. However, we can still give sufficient conditions for the existence of a positive spectrum for L_0^{qcf}.

We now consider the case of finite-range interactions and assume that

$$\begin{aligned} \phi''_{rF} &\leq 0 \quad \text{for } 2 \leq r \leq R-1, \\ \phi''_{RF} &< 0. \end{aligned} \tag{4.1}$$

In this section we will show that $L^{\mathrm{a}} - L^{\mathrm{c}}$ is positive semidefinite and derive bounds on its positive square root. This will allow us to show that L_0^{qcf} is similar to a symmetric, positive semidefinite matrix and to give bounds on the condition number of the matrix of eigenvectors.

REMARK 4.1. *We note that $\phi''_{rF} \leq 0$ for $r > 1$ is a common assumption. For many of the common pair interaction potentials, such as the Lennard-Jones potential, $\phi(r) = Ar^{-12} + Br^{-6}$, or the Morse potential, $\phi(r) = \exp(-2\alpha(r - r_0)) + 2\exp(-\alpha(r - r_0))$, there exists a minimal strain F_* such that, for all $F \geq F_*$, we have $\phi''_{rF} \leq 0$ for $r = 2, \ldots, R$. In most cases, it is reasonable to assume that the macroscopic strain F remains in this region, as it would require extreme compressive forces to violate it. The second condition is equivalent to stating that not all ϕ''_{rF} are zero for $r > 1$ (i.e., that we are not in the nearest neighbor interaction case).*

4.1. Symmetrization of L^{qcf}. We write the atomistic and continuum operators in terms of Laurent polynomials of the translation operator. This allows us to show that $L^{\mathrm{a}} - L^{\mathrm{c}}$ is positive semidefinite (Lemma 4.1), to factor $Y = (L^{\mathrm{a}} - L^{\mathrm{c}})^{1/2}$ as $Y = L\tilde{Y}$, where $\tilde{Y}$ is invertible, and to derive bounds on $||\tilde{Y}^{-1}||$ in terms of the interaction coefficients (Lemma 4.2). In terms of the translation operator defined in (2.5), we can express L^{a} and L^{c} as

$$L^{\mathrm{c}} = \sum_{r=1}^{R} r^2 \phi''_{rF}\left[-T + 2I - T^{-1}\right] \quad \text{and} \quad L^{\mathrm{a}} = \sum_{r=1}^{R} \phi''_{rF}\left[-T^r + 2I - T^{-r}\right]. \tag{4.2}$$

We write the difference $L^{\mathrm{a}} - L^{\mathrm{c}}$ as a Laurent polynomial of the translation operator T:

$$\begin{aligned} L^{\mathrm{a}} - L^{\mathrm{c}} &= \sum_{r=2}^{R} \phi''_{rF}\left[(-T^r + 2I - T^{-r}) - r^2(-T + 2I - T^{-1})\right] \\ &= \sum_{r=2}^{R} \phi''_{rF}\left[(T^r - I)(T^{-r} - I) - r^2(T - I)(T^{-1} - I)\right]. \end{aligned}$$

Thus, if we define the Laurent polynomial

$$b(t) = \sum_{r=2}^{R} \phi''_{rF}\left[(t^r - 1)(t^{-r} - 1) - r^2(t - 1)(t^{-1} - 1)\right] \quad \text{for } t \in \mathbb{C} \setminus \{0\}, \tag{4.3}$$

then we obtain $L^{\mathrm{a}} - L^{\mathrm{c}} = b(T)$. Since the spectrum of the translation operator (2.6) is contained in the unit circle $\mathcal{T}$, we may show that $L^{\mathrm{a}} - L^{\mathrm{c}} \geq 0$ by showing that $b(t) \geq 0$ for $|t| = 1$. We will use the form of $b(t)$ in the following to derive bounds on the square root $(L^{\mathrm{a}} - L^{\mathrm{c}})^{1/2}$ and eventually on the matrix of eigenvectors.

LEMMA 4.1. *Suppose that* (4.1) *holds; then* $b(t) \geq 0$ *in* $\mathcal{T}$. *In particular,* $L^{\mathrm{a}} - L^{\mathrm{c}}$ *is positive semidefinite.*

Proof. Rewrite $b(t)$ in the form

$$b(t) = \sum_{r=2}^{R} b_{(r)}(t), \tag{4.4}$$

where

$$\begin{aligned} b_{(r)}(t) &:= \phi''_{rF}\big[(t^r - 1)(t^{-r} - 1) - r^2(t-1)(t^{-1}-1)\big] \\ &= \phi''_{rF}(t-1)(t^{-1}-1)\big[(t^{r-1} + t^{r-2} + \cdots + 1)(t^{-r+1} + t^{-r+2} + \cdots + 1) - r^2\big]. \end{aligned} \tag{4.5}$$

It is easy to see that $(t-1)(t^{-1}-1)$ is nonnegative on $\mathcal{T}$, and, moreover, for $t \in \mathcal{T}$,

$$(t^{r-1} + t^{r-2} + \cdots + 1)(t^{-r+1} + t^{-r+2} + \cdots + 1) = |t^{r-1} + t^{r-2} + \cdots + 1|^2 \leq r^2. \tag{4.6}$$

Hence, due to (4.1),

$$b_{(r)}(t) \geq 0 \quad \text{on } \mathcal{T} \quad \text{for } r = 2, \ldots, R, \tag{4.7}$$

and we therefore obtain the stated result. ∎

Since $L^{\mathrm{a}} - L^{\mathrm{c}}$ is symmetric, positive semidefinite, it has a unique symmetric, positive semidefinite square root, which we denote by

$$Y = (L^{\mathrm{a}} - L^{\mathrm{c}})^{1/2}. \tag{4.8}$$

While Y is not an invertible matrix, we will define a modified operator that is equivalent when restricted to $\mathcal{U}$. We will then use this modified operator as a similarity transform for L^{qcf}.

LEMMA 4.2. *Suppose that* (4.1) *holds; then there exists a symmetric, positive definite* $\tilde{Y}$ *such that* $L^{\mathrm{a}} - L^{\mathrm{c}} = \tilde{Y}^2 L^2$. *Moreover, the bounds*

$$\|\tilde{Y}\| \leq \beta_1 \quad \textit{and} \quad \|\tilde{Y}^{-1}\| \leq 1/\beta_0, \tag{4.9}$$

for $0 < \beta_0 < \beta_1$, *are independent of* N *and* $\mathcal{A}$.

Proof. We work with the polynomial representation, $b(T) = L^{\mathrm{a}} - L^{\mathrm{c}}$, in order to factor the operator. It can be immediately seen from the definition of $b(t)$ that $b(1) = 0$ and, since $b(t) = b(1/t)$, $t = 1$ is at least a double root of $b(t)$. Upon dividing $b(t)$ by $(t-1)(t^{-1}-1)$ we obtain

$$\begin{aligned} b_1(t) &:= \frac{b(t)}{(t-1)(t^{-1}-1)} \\ &= \sum_{r=2}^{R} \phi''_{rF}\big[(1 + t + \cdots + t^{r-1})(1 + t^{-1} + \cdots + t^{-r+1}) - r^2\big], \end{aligned} \tag{4.10}$$

and hence $b_1(1) = 0$. Since $b_1(t) = b_1(1/t)$, $t = 1$ is again at least a double root and

$$\tilde{b}(t) := \frac{b_1(t)}{(t-1)(t^{-1}-1)} = \frac{b(t)}{(t-1)^2(t^{-1}-1)^2}$$

is a proper Laurent polynomial.

Since $b(t)$ and $(t-1)^2(t^{-1}-1)^2$ are nonnegative for $|t|=1$, $\tilde{b}(t)$ is also nonnegative for $|t|=1$. Since the spectrum of T (2.6) lies in $\mathcal{T}$, this implies that $\tilde{b}(T) \geq 0$, and we can thus define the square root of the operator $\tilde{b}(T)$,

$$\tilde{Y} = (\tilde{b}(T))^{1/2}. \tag{4.11}$$

Thus, we obtain

$$L^{\mathrm{a}} - L^{\mathrm{c}} = b(T) = \tilde{b}(T)\,(T-1)^2(T^{-1}-1)^2 = \tilde{Y}^2\,L^2.$$

The constants β_0 and β_1 in (4.9) are defined as

$$\beta_0^2 := \min_{t\in\mathcal{T}} \tilde{b}(t) \quad \text{and} \quad \beta_1^2 := \max_{t\in\mathcal{T}} \tilde{b}(t),$$

and they obviously do not depend on N and $\mathcal{A}$. It remains only to show strict positivity of β_0.

Suppose that $\tilde{b}(t_1) = 0$ at some point $t_1 \in \mathcal{T}$. Then $b(t_1) = 0$ and hence, in view of (4.4) and (4.7), each $b_{(r)}(t_1) = 0$. We write the longest-range term:

$$b_{(R)}(t_1) = (-\phi''_{RF})\big[R^2(t_1-1)(t_1^{-1}-1) - (t_1^R-1)(t_1^{-R}-1)\big] = 0.$$

It follows from (4.5) and (4.6) that this may happen only at $t_1 = 1$. However, a straightforward computation shows that

$$\begin{aligned}\tilde{b}(1) = &\sum_{r=2}^{R}(-\phi''_{rF}) \lim_{t\to 1} \frac{r^2(t-1)(t^{-1}-1) - (t^r-1)(t^{-r}-1)}{\big[(t-1)(t^{-1}-1)\big]^2} \\ \geq\ & (-\phi''_{RF}) \lim_{t\to 1} \frac{R^2(t-1)(t^{-1}-1) - (t^R-1)(t^{-R}-1)}{\big[(t-1)(t^{-1}-1)\big]^2} \geq (-\phi''_{RF})\frac{R^4-R^2}{12} > 0.\end{aligned}$$

Hence no point $t_1 \in \mathcal{T}$ such that $\tilde{b}(t_1) = 0$ exists, which implies that $\beta_0 > 0$. ∎

REMARK 4.2. *In our preprint* [9] *we prove a sharper bound on* β_0, β_1*: If* (4.1) *holds, then* (4.9) *holds with constants*

$$\beta_0^2 = \sum_{r=2}^{R}(-\phi''_{rF})\frac{2r^2+(-1)^r-1}{8} \quad \textit{and} \quad \beta_1^2 = \sum_{r=2}^{R}(-\phi''_{rF})\frac{r^2(r^2-1)}{12}.$$

The lower bound is attained at $t=-1$ *and the upper bound is attained at* $t=1$.

We will not use this result in the remainder of the paper.

Using Lemma 4.2, we may write the QCF operator as

$$L^{\mathrm{qcf}} = L^{\mathrm{c}} + X\tilde{Y}^2L^2 \quad \text{and} \quad L_0^{\mathrm{qcf}} = L^{\mathrm{c}} + P_{\mathcal{U}}X\tilde{Y}^2L^2. \tag{4.12}$$

As a consequence of Lemma 4.2, we see that Y is always singular. Nevertheless, we may construct a similarity transformation to diagonalize L_0^{qcf} by simply replacing L by its invertible variant L_1 defined in (2.4).

PROPOSITION 4.3. *Suppose that* (4.1) *holds and that* $W_F'' > 0$. *Let* $Y = L\tilde{Y}$, *where* $\tilde{Y}$ *is defined in Lemma* 4.2*; then* L_0^{qcf} *is similar to a symmetric, positive semi-definite matrix,*

$$L^{\mathrm{sym}} := (\tilde{Y}L_1)L_0^{\mathrm{qcf}}(\tilde{Y}L_1)^{-1} = L^{\mathrm{c}} + YXY, \tag{4.13}$$

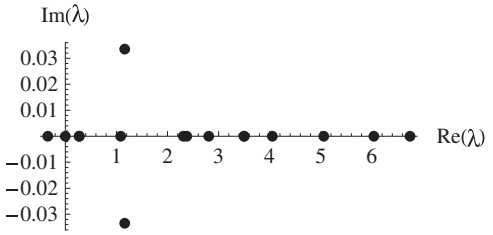

FIG. 4.1. *Spectrum of* $L_0^{\rm qcf}$ *for* $N = 16$, $\mathcal{A} = \{1, 2, \ldots, 8\}$, $R = 3$, $\varphi_F'' = 0$, $\varphi_{2F}'' = 1$, $\varphi_F'' = -1/4$. *We see that the spectrum is not real, which shows that QCF cannot have the spectrum identical to that of an energy-based method for* $R \geq 3$.

and hence is diagonalizable with a real, nonnegative spectrum. Moreover, $L_0^{\rm qcf}$ *is positive definite on* $\mathcal{U}$.

Proof. We first use Lemma 4.2 to represent $L^{\rm a} - L^{\rm c}$. Moreover, we recall that $\tilde{Y}$ commutes with T and thus other polynomials in T such as L. We use the fact that $P_{\mathcal{U}} L_1 = L_1 P_{\mathcal{U}} = L$ and likewise that $L_1 L = L L_1 = L^2$ to obtain

$$\begin{aligned}
[\tilde{Y} L_1] L_0^{\rm qcf} &= [\tilde{Y} L_1] L^{\rm c} + \tilde{Y} [L_1 P_{\mathcal{U}}] X \tilde{Y}^2 L^2 \\
&= L^{\rm c} [\tilde{Y} L_1] + \tilde{Y} L X \tilde{Y}^2 L L_1 \\
&= [L^{\rm c} + \tilde{Y} L X \tilde{Y} L]\, [\tilde{Y} L_1].
\end{aligned}$$

To show that $L^{\rm sym}$ is positive semidefinite on $\mathbb{R}^N$ and positive definite on $\mathcal{U}$, we note that

$$\langle L^{\rm sym} u, u \rangle = \langle L^{\rm c} u, u \rangle + \langle XYu, Yu \rangle \geq W_F'' \langle Lu, u \rangle. \qquad \square$$

REMARK 4.3. *If we remove condition* (4.1), *then we can no longer ensure that* $b(t) \geq 0$. *One can still define a complex symmetric matrix* $Y = (L^{\rm a} - L^{\rm c})^{1/2}$ *such that* $Y L_0^{\rm qcf} = [L^{\rm c} + YXY] Y$. *However, in this case* $L_0^{\rm qcf}$ *does not necessarily have a real spectrum.*

For instance, if $R = 3$ *and* $\phi_{3F}'' = -\frac{1}{4}\phi_{2F}''$, *then a straightforward calculation yields the spectrum of* $L^{\rm a} - L^{\rm c}$ *being*

$$\left\{ 8 \cos\left(\tfrac{2\pi k}{N}\right) \sin^4\left(\tfrac{\pi k}{N}\right) : k = 0, 1, \ldots, N-1 \right\},$$

which is seen to have both positive and negative eigenvalues.

Further, we plot the spectrum of $L_0^{\rm qcf}$ *for* $N = 16$, $\mathcal{A} = \{1, 2, \ldots, 8\}$, $R = 3$, $\phi_F'' = 0$, $\phi_{2F}'' = 1$, $\phi_{3F}'' = -1/4$ *in Figure* 4.1. *We see that the spectrum of* $L_0^{\rm qcf}$ *is indeed not real. This observation shows that there is no energy-based method for* $R \geq 3$ *whose spectrum always coincides with the spectrum of QCF, since an operator of an energy-based method is always symmetric with a real spectrum.*

In Figure 4.2 *we confirm numerically that even for parameter values satisfying our theorem, the positive spectrum is generally different from the standard generalizations of the operator* $L^{\rm qnl}$ *to further neighbors* [10, 13, 20].

4.2. Condition number of the ℓ^2-eigenbasis. According to Proposition 4.3, $L_0^{\rm qcf}$ and $L^{\rm sym}$ are similar matrices. Since $L^{\rm sym}$ is real and symmetric, there exists an orthonormal operator $V^{\rm sym} \in \mathbb{R}^{N \times N}$ such that

$$L^{\rm sym} = V^{\rm sym} \Lambda [V^{\rm sym}]^T,$$

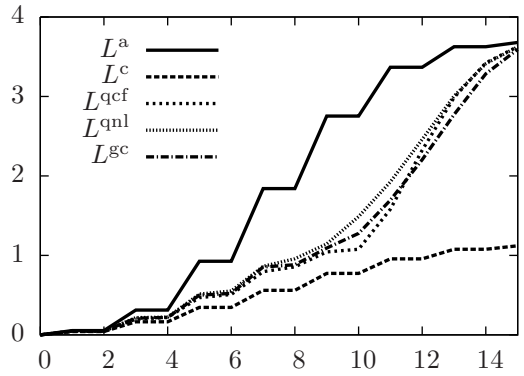

FIG. 4.2. *We plot the spectrum of* $L^{\mathrm{a}}, L^{\mathrm{c}}, L_0^{\mathrm{qcf}}, L^{\mathrm{qnl}}, L^{\mathrm{gc}}$ *for* $N = 16$, $\mathcal{A} = \{1, 2, \ldots, 8\}$, $R = 3$, $\phi_F'' = 1$, $\phi_{2F}'' = 0$, $\phi_{3F}'' = -0.08$, *where* L^{gc} *denotes the geometrically consistent scheme of* [10]. *We see that the spectrum of the QCF operator is generally different from the generalizations of QNL. We note the ordering of the spectra as shown in Theorem* 4.7.

where Λ is the diagonal matrix of eigenvalues of L_0^{qcf}, and we obtain

$$L_0^{\mathrm{qcf}} = [\tilde{Y}^{-1} L_1^{-1} V^{\mathrm{sym}}] \Lambda [\tilde{Y}^{-1} L_1^{-1} V^{\mathrm{sym}}]^{-1};$$

that is, the operator $\tilde{Y}^{-1} L_1^{-1} V^{\mathrm{sym}}$ diagonalizes L_0^{qcf}. As in the nearest neighbor case, the eigenbasis $\tilde{Y}^{-1} L_1^{-1} V^{\mathrm{sym}}$ is poorly scaled and would lead to an $O(N^2)$ condition number. However, the same argument as in Remark 3.1 shows how to rescale the basis to obtain the following theorem.

THEOREM 4.4. *Suppose that* (4.1) *holds, and let* $\tilde{Y}$ *be defined by* (4.11). *Then the operator* $V^{\mathrm{qcf}} \in \mathbb{R}^{N \times N}$,

$$V^{\mathrm{qcf}} = \left[W_F'' \tilde{Y}^{-1} + P_{\mathcal{U}} X \tilde{Y} L \right] V^{\mathrm{sym}},$$

diagonalizes L_0^{qcf}, *that is,* $L_0^{\mathrm{qcf}} V^{\mathrm{qcf}} = V^{\mathrm{qcf}} \Lambda$, *where* Λ *is a diagonal real matrix of eigenvalues.*

Moreover, if $W_F'' > 0$, *then* L_0^{qcf} *is positive definite on* $\mathcal{U}$, V^{qcf} *is invertible, and* $\mathrm{cond}(V^{\mathrm{qcf}})$ *is bounded above by a constant that depends only on* W_F'', β_0, β_1 *and, in particular, is independent of* N *and* $\mathcal{A}$.

Proof. The proof of this result is very similar to the proof of Theorem 3.3, and hence we shall be fairly brief. First, we note that, due to (4.9), the matrix $\tilde{Y}$ is invertible, and hence V^{qcf} is well defined. Moreover, we recall that $\tilde{Y}$ commutes with L.

Step 1: *Diagonalization.* Using the definitions of L_0^{qcf} in (4.12) and L^{sym} in (4.13), we obtain

$$\begin{aligned} L_0^{\mathrm{qcf}} V^{\mathrm{qcf}} &= \left[W_F'' L + P_{\mathcal{U}} X \tilde{Y}^2 L^2 \right] \left[W_F'' \tilde{Y}^{-1} + P_{\mathcal{U}} X \tilde{Y} L \right] V^{\mathrm{sym}} \\ &= \left[W_F'' \tilde{Y}^{-1} + P_{\mathcal{U}} X \tilde{Y} L \right] \left[W_F'' L + L \tilde{Y} P_{\mathcal{U}} X \tilde{Y} L \right] V^{\mathrm{sym}} \\ &= \left[W_F'' \tilde{Y}^{-1} + P_{\mathcal{U}} X \tilde{Y} L \right] V^{\mathrm{sym}} \Lambda \\ &= V^{\mathrm{qcf}} \Lambda. \end{aligned}$$

Step 2: *Estimating* $\mathrm{cond}(V^{\mathrm{qcf}})$. Suppose now that $W_F'' > 0$. As before, bounding $\|V^{\mathrm{qcf}}\|$ is straightforward. Using Lemma 4.2, we obtain

$$\|V^{\mathrm{qcf}}\| \le W_F''\|\tilde{Y}^{-1}\| + \|P_{\mathcal{U}}X\tilde{Y}L\| \le W_F''/\beta_0 + 4\beta_1. \tag{4.14}$$

To bound $\|[V^{\mathrm{qcf}}]^{-1}\|$, we will use the fact that $\|[V^{\mathrm{qcf}}]^{-1}\| = \|[V^{\mathrm{qcf}}]^{-T}\|$ and show that

$$\|[V^{\mathrm{qcf}}]^T u\| \ge \tilde{\gamma}_0\|u\| \qquad \forall u \in \mathbb{R}^N. \tag{4.15}$$

To prove (4.15), we rewrite V^{qcf} as

$$V^{\mathrm{qcf}} = \left[I + \tfrac{1}{W_F''}P_{\mathcal{U}}X\tilde{Y}L\tilde{Y}\right]\left[W_F''\tilde{Y}^{-1}V^{\mathrm{sym}}\right].$$

Setting $\alpha = -1/W_F'' \le 0$, $Z = \tilde{Y}$, we can apply Lemma 4.6 to deduce that there exists a constant γ_0, which depends only on $\alpha\|Z\|^2 = -\beta_1^2/W_F''$, such that

$$\left\|[V^{\mathrm{qcf}}]^T u\right\| \ge \gamma_0\left\|\left[W_F''\tilde{Y}^{-1}V^{\mathrm{sym}}\right]u\right\| \ge \frac{W_F''\gamma_0}{\beta_1}\|u\|;$$

that is, (4.15) is indeed true with $\tilde{\gamma}_0 = W_F''\gamma_0/\beta_1$.

Combining (4.14) and (4.15) gives the stated result. ∎

LEMMA 4.5. *Let $A = I + P_{\mathcal{U}}XB$, where $B \in \mathbb{R}^{N\times N}$ is symmetric, $B + I \ge \gamma I$ with $\gamma > 0$, and $P_{\mathcal{U}}B = B$. Then there exists a constant $\gamma_0 > 0$, depending only on γ and $\|B\|$, such that*

$$\|A^T u\| \ge \gamma_0\|u\| \qquad \forall u \in \mathbb{R}^N.$$

Proof. We decompose A^T into

$$A^T = I + BXP_{\mathcal{U}} = \left[I - P_{\mathcal{U}}\right] + P_{\mathcal{U}}\left[I + BXP_{\mathcal{U}}\right],$$

where we have used the fact that $P_{\mathcal{U}}B = B$. Since $P_{\mathcal{U}}$ is an orthogonal projection, we obtain, again using $P_{\mathcal{U}}B = B$,

$$\|A^T v\|^2 = \|[I - P_{\mathcal{U}}]v\|^2 + \|[I + BX]P_{\mathcal{U}}v\|^2. \tag{4.16}$$

We will show next that

$$\|[I + BX]w\|^2 \ge (1 - \epsilon)\|w\|^2 \qquad \forall w \in \mathcal{U}, \tag{4.17}$$

where $\epsilon \in (0, 1)$ is defined in (4.21) and depends only on the smallest and largest eigenvalues of B but not on N or $\mathcal{A}$. Hence, (4.17) combined with (4.16) gives the desired result,

$$\|A^T v\|^2 \ge (1 - \epsilon)(\|[1 - P_{\mathcal{U}}]v\|^2 + \|P_{\mathcal{U}}v\|^2) = \gamma_0\|v\|^2,$$

with $\gamma_0 = \sqrt{1 - \epsilon}$.

Proof of (4.17). We begin by splitting the operator, using $X^2 = X$, into

$$\begin{aligned}[I + BX] &= X[I + BX] + [I - X][I + BX] \\ &= X[I + B]X + [I - X][I + BX] \\ &=: S_1 + S_2.\end{aligned}$$

Since X is an orthogonal projection, we have, for any $w \in \mathcal{U}$,

$$\big\|[I+BX]w\big\|^2 = \|S_1 w\|^2 + \|S_2 w\|^2. \tag{4.18}$$

Estimating S_1. Since $S_1 = X[I+B]X$ is a symmetric operator, we have the following variational bound:

$$\big\langle X[I+B]Xw, w\big\rangle = \big\langle (I+B)Xw, Xw\big\rangle \geq \gamma \|Xw\|,$$

which leads to the following $N, \mathcal{A}$-independent bound:

$$\|S_1 w\|^2 \geq \gamma^2 \|Xw\|^2 \qquad \forall w \in \mathbb{R}^N. \tag{4.19}$$

Estimating S_2. Due to the good estimate on S_1 we need only fairly rough estimates on the term $\|S_2 w\|^2$. Application of the Cauchy–Schwarz inequality and a weighted Cauchy inequality provides the estimate

$$\|S_2 w\|^2 \geq (1-\epsilon)\|[I-X]w\|^2 + (1-\epsilon^{-1})\|[I-X]BXw\|^2$$

for any $\epsilon \in (0,1)$. Using the fact that $I - X$ is an orthogonal projection, we can further estimate

$$\|S_2 w\|^2 \geq (1-\epsilon)\|[I-X]w\|^2 + (1-\epsilon^{-1})\|B\|^2\|Xw\|^2. \tag{4.20}$$

Combining the estimates. Inserting (4.19) and (4.20) into (4.18), we obtain, for all $w \in \mathcal{U}$,

$$\begin{aligned} \|[I-\alpha Z^T L Z X]w\|^2 \geq\ & \big\{\gamma^2 + (1-\epsilon^{-1})\|B\|^2\big\}\|Xw\|^2 + (1-\epsilon)\|[I-X]w\|^2 \\ \geq\ & \min\big\{\gamma^2 + (1-\epsilon^{-1})\|B\|^2, 1-\epsilon\big\}\|w\|^2 \end{aligned}$$

for any $\epsilon \in (0,1)$. It is clear that choosing ϵ sufficiently close to 1 gives a positive lower bound. To optimize this constant with respect to ϵ, we have to choose ϵ to equalize the two competitors in the min expression. The resulting choice is

$$\epsilon = \tfrac{1}{2}\Big(1 - \|B\|^2 - \gamma^2 + \sqrt{4\|B\|^2 + (\|B\|^2 - 1 + \gamma^2)^2}\Big), \tag{4.21}$$

which concludes the proof of (4.17). (As a matter of interest, $\epsilon \to 1$ as $\|B\| \to \infty$ or $\gamma \to 0$, and $\epsilon = 0$ for $B = 0$.) ∎

LEMMA 4.6. *Let $A = I - \alpha P_{\mathcal{U}} X Z^T L Z$, where $Z \in \mathbb{R}^{N\times N}$ commutes with $P_{\mathcal{U}}$ and where $\alpha \in \mathbb{R}$ satisfies*

$$-\infty < \alpha \|Z\|^2 < 1/4;$$

then there exists a constant $\gamma_0 > 0$, depending only on $\alpha\|Z\|^2$, such that

$$\|A^T u\| \geq \gamma_0 \|u\| \qquad \forall u \in \mathbb{R}^N. \tag{4.22}$$

Proof. We choose $B = -\alpha Z^T L Z$ in Lemma 4.5. We can estimate

$$\|B\| \leq |\alpha|\|L\|\|Z\|^2 \leq 4|\alpha|\|Z\|^2.$$

One can see that B is positive definite if $\alpha < 0$ and $\|B\| \leq 4\alpha\|Z\|^2 < 1$, which implies that $B + I \geq (1 - 4\alpha\|Z\|^2)I$ if $\alpha \geq 0$. Hence all the conditions of Lemma 4.5 are satisfied and (4.22) holds with γ_0 depending only on $\alpha\|Z\|^2$. ∎

4.3. Estimates for the eigenvalues. Using the similarity to a symmetric matrix that we have established in the previous section we can now give sharp bounds on the spectrum of $L_0^{\rm qcf}$.

THEOREM 4.7. *Suppose that* (4.1) *holds; then* $L_0^{\rm qcf}$ *has a real, ordered spectrum* $(\lambda_j)_{j=1}^N$. *If we denote the ordered eigenvalues of* $L^{\rm a}$ *and* $L^{\rm c}$, *respectively, by* $(\lambda_j^{\rm a})_{j=1}^N$ *and* $(\lambda_j^{\rm c})_{j=1}^N$, *then*

$$\lambda_j^{\rm c} \le \lambda_j \le \lambda_j^{\rm a} \qquad \text{for } j = 1, \dots, N.$$

Proof. We know from Theorem 4.4 that $L_0^{\rm qcf}$ is diagonalizable and that it is similar to the self-adjoint operator $L^{\rm sym}$ defined in (4.13), which has a real spectrum that is identical to the spectrum of $L_0^{\rm qcf}$. We will next show that, for all $u \in \mathbb{R}^N$,

$$\langle L^{\rm c} u, u\rangle \le \langle L^{\rm sym} u, u\rangle \le \langle L^{\rm a} u, u\rangle. \tag{4.23}$$

From these inequalities, the min-max characterization of eigenvalues [18, sect. XIII.1] immediately gives the stated result.

To prove (4.23) we will take the following starting point:

$$\langle L^{\rm sym} u, u\rangle = \langle L^{\rm c} u, u\rangle + \langle Y^T X Y u, u\rangle = \langle L^{\rm c} u, u\rangle + \langle X Y^T u, X Y^T u\rangle. \tag{4.24}$$

Using (4.24) and the fact that $Y^T Y = L^{\rm a} - L^{\rm c}$, we have

$$\langle L^{\rm sym} u, u\rangle \le \langle L^{\rm c} u, u\rangle + \langle Y^T u, Y^T u\rangle = \langle L^{\rm c} u, u\rangle + \langle [L^{\rm a} - L^{\rm c}] u, u\rangle = \langle L^{\rm a} u, u\rangle.$$

For the lower bound we use (4.24) and the fact that $\langle X Y^T u, X Y^T u\rangle$ is nonnegative to obtain

$$\langle L^{\rm sym} u, u\rangle \ge \langle L^{\rm c} u, u\rangle. \qquad \square$$

REMARK 4.4. *The assumptions in* (4.1) *can be slightly weakened. In our preprint* [9], *we require only that the polynomial* $b(t)$ *defined in* (4.3) *not change sign. It would be interesting to know a general characterization of coefficients* ϕ''_{rF} *that guarantees that* $b(t)$ *does not change sign. All results can, with some minor additional technicalities and additional assumptions, be extended to this case. If* $b(t)$ *were nonpositive, then the result of Theorem* 4.7 *would, instead, read as* $\lambda_j^{\rm a} \le \lambda_j \le \lambda_j^{\rm c}$.

5. Applications of the spectral analysis. In this final section we present two further interesting applications of our foregoing analysis. First, we discuss the GMRES solution of a linearized QCF system. Second, we prove a new stability result for the linearized QCF operator in a discrete Sobolev norm, which we hope will become a useful tool for future analyses of the QCF method.

Our results in this section are fairly straightforward corollaries or extensions from our ℓ^2-analysis in section 4; in particular, the techniques used to analyze the ℓ^2-eigenvalue problem immediately apply to the generalized eigenvalue problems we discuss in section 5.1. Hence, we will keep our presentation in this section less formal.

5.1. GMRES solution of the QCF system. We consider the linearized QCF system

$$L_0^{\rm qcf} u = f, \tag{5.1}$$

where $f \in \mathcal{U}$, which is to be solved for $u \in \mathcal{U}$. Since $L_0^{\rm qcf}$ in nonsymmetric, the GMRES algorithm is a reasonable choice for solving the linearized QCF equations (see [19] for

a general introduction and [8] for a detailed discussion of using GMRES for solving the QCF system). We recall that the GMRES algorithm is an iterative scheme that selects an approximate solution u^m by minimizing the norm of the residual,

$$u^m = \arg\min_{v \in \mathcal{K}_m} ||L_0^{\mathrm{qcf}} v - f||,$$

in the Krylov subspace $\mathcal{K}_m = \mathrm{span}\{f, L_0^{\mathrm{qcf}} f, (L_0^{\mathrm{qcf}})^2 f, \ldots, (L_0^{\mathrm{qcf}})^{m-1} f\}$. Standard estimates on GMRES convergence [19], along with the analysis of the previous sections, show that the residual of the mth iterate, $r^{(m)} = f - L_0^{\mathrm{qcf}} u^{(m)}$, satisfies the bound

$$\|r^{(m)}\| \le 2\,\mathrm{cond}(V^{\mathrm{qcf}}) \left(\frac{1-\sqrt{\gamma}}{1+\sqrt{\gamma}}\right)^m \|r^{(0)}\|, \tag{5.2}$$

where $\gamma = \lambda_2/\lambda_N = O(1/N^2)$ (see also [8, Prop. 22]). The fraction λ_2/λ_N is used instead of λ_1/λ_N since we are solving the system in $\mathcal{U}$.

The above convergence is rather slow, and hence two variants of preconditioned GMRES (P-GMRES) algorithms were suggested in [8]. In both cases, the preconditioner used was the negative Laplacian L. We will use the preconditioner L_1 instead of L; however, this is purely for the sake of a consistent notation since on $\mathcal{U}$ we have $L_1^{-1} L_0^{\mathrm{qcf}} = L^{-1} L_0^{\mathrm{qcf}}$ (note that $\mathrm{rg}\, L_0^{\mathrm{qcf}} = \mathcal{U}$ and that L^{-1} is well defined on $\mathcal{U}$).

The first variant of P-GMRES that was considered in [8] was the standard left-preconditioned GMRES algorithm where GMRES is applied to the system

$$L_1^{-1} L_0^{\mathrm{qcf}} u = L_1^{-1} f. \tag{5.3}$$

That is, we define the approximate solution

$$u^m = \arg\min_{v \in \widetilde{\mathcal{K}}_m} ||L_1^{-1}(L_0^{\mathrm{qcf}} v - f)||,$$

where

$$\widetilde{\mathcal{K}}_m = \mathrm{span}\{L_1^{-1} f, (L_1^{-1} L_0^{\mathrm{qcf}}) L_1^{-1} f, (L_1^{-1} L_0^{\mathrm{qcf}})^2 L_1^{-1} f, \ldots, (L_1^{-1} L_0^{\mathrm{qcf}})^{m-1} L_1^{-1} f\}. \tag{5.4}$$

To obtain convergence rates, we require bounds on the eigenvalues and eigenbasis of $L_1^{-1} L_0^{\mathrm{qcf}}$, which we derive below.

The second variant again considers the left-preconditioned system (5.3), but this time the residual is minimized in the norm induced by the operator L_1,

$$u^m = \arg\min_{v \in \widetilde{\mathcal{K}}_m} ||L_1^{-1/2}(L_0^{\mathrm{qcf}} v - f)||,$$

where $\widetilde{\mathcal{K}}_m$ is defined in (5.4). The convergence rates of the resulting method are governed by the spectrum and eigenbasis of the operator $L_1^{-1/2} L_0^{\mathrm{qcf}} L_1^{-1/2}$, which we derive below.

REMARK 5.1. *Both of these variants were proposed in* [8] *and analyzed using the (at the time) numerically observed spectral properties of* L_0^{qcf}. *Here, we give results that are now justified rigorously. The results benefit from sharper bounds on the condition number of the matrices of eigenvectors, which leads to better convergence estimates for the proposed algorithms.*

5.1.1. Diagonalization. We consider $L_1^{-1/2} L_0^{\mathrm{qcf}} L_1^{-1/2}$ first. Using the fact that $L_1^{-1/2}$ commutes with $L_1 \tilde{Y}$, we obtain

$$[L_1\tilde{Y}][L_1^{-1/2} L_0^{\mathrm{qcf}} L_1^{-1/2}][L_1\tilde{Y}]^{-1} = L_1^{-1/2} L^{\mathrm{sym}} L_1^{-1/2} = \tilde{V}^{\mathrm{sym}} \tilde{\Lambda} (\tilde{V}^{\mathrm{sym}})^T,$$

where $\tilde{\Lambda}$ is the real diagonal matrix of eigenvalues and $\tilde{V}^{\mathrm{sym}}$ an orthonormal matrix of eigenvectors of the symmetric operator $L_1^{-1/2} L^{\mathrm{sym}} L_1^{-1/2}$. By similarity of the matrices, we conclude that $L_1^{-1/2} L_0^{\mathrm{qcf}} L_1^{-1/2}$ is diagonalizable with real spectrum $\tilde{\Lambda}$:

$$[L_1^{-1/2} L_0^{\mathrm{qcf}} L_1^{-1/2}][\tilde{Y}^{-1} L_1^{-1} \tilde{V}^{\mathrm{sym}}] = [\tilde{Y}^{-1} L_1^{-1} \tilde{V}^{\mathrm{sym}}]\tilde{\Lambda}. \tag{5.5}$$

Multiplying the equation by $L_1^{-1/2}$, we obtain

$$[L_1^{-1} L_0^{\mathrm{qcf}}][\tilde{Y} L_1^{-3/2} \tilde{V}^{\mathrm{sym}}] = [\tilde{Y}^{-1} L_1^{-3/2} \tilde{V}^{\mathrm{sym}}]\tilde{\Lambda}, \tag{5.6}$$

thus showing that also $L_1^{-1} L_0^{\mathrm{qcf}}$ is diagonalizable with the same real spectrum $\tilde{\Lambda}$.

5.1.2. Eigenvalue bounds. To establish convergence rates for the P-GMRES solution of the QCF system, we need to obtain bounds on the eigenvalues contained in $\tilde{\Lambda}$. Let $(\tilde{\lambda}_n)_{n=1}^N$ denote the ordered eigenvalues of $\tilde{\Lambda}$, and let $(\tilde{\lambda}_n^{\mathrm{a}})_{n=1}^N$ and $(\tilde{\lambda}_n^{\mathrm{c}})_{n=1}^N$ denote, respectively, the ordered eigenvalues of $L_1^{-1/2} L^{\mathrm{a}} L_1^{-1/2}$ and $L_1^{-1/2} L^{\mathrm{c}} L_1^{-1/2}$. Since $L^{\mathrm{c}} = W_F'' L$, we know that

$$\tilde{\lambda}_1^{\mathrm{c}} = 0 \quad \text{and} \quad \tilde{\lambda}_n^{\mathrm{c}} = W_F'' \quad \text{for } n = 2, \dots, N.$$

Replacing u by $L_1^{-1/2} u$ in (4.23), we obtain that

$$\left\langle [L_1^{-1/2} L^{\mathrm{c}} L_1^{-1/2}]u, u \right\rangle \le \left\langle [L_1^{-1/2} L^{\mathrm{sym}} L_1^{-1/2}]u, u \right\rangle \le \left\langle [L_1^{-1/2} L^{\mathrm{a}} L_1^{-1/2}]u, u \right\rangle \qquad \forall u \in \mathcal{U}.$$

Hence, we can repeat the proof of Theorem 4.7 verbatim to show that

$$\tilde{\lambda}_j^{\mathrm{c}} \le \tilde{\lambda}_j \le \tilde{\lambda}_j^{\mathrm{a}} \qquad \text{for } j = 1, \dots, N.$$

At this point we need to make an assumption on the stability of the atomistic system. We assume that the macroscopic strain F is chosen so that $W_F'' > 0$, from which we deduce that

$$W_F'' \le \tilde{\lambda}_j \le \sum_{r=1}^{R} |\phi_{rF}''| r^2 \qquad \text{for } j = 2, \dots, N,$$

which are bounds that are independent of N and $\mathcal{A}$.

5.1.3. Condition number bounds. Using the fact that $\tilde{V}^{\mathrm{sym}}$ is orthogonal and using Lemma 4.2 to bound $\mathrm{cond}(\tilde{Y}) \le \beta_1/\beta_0$, we can obtain the following upper bounds on the condition number of the matrices of eigenvectors:

$$\mathrm{cond}(\tilde{Y}^{-1} L_1^{-1} \tilde{V}^{\mathrm{sym}}) \le \mathrm{cond}(\tilde{Y})\,\mathrm{cond}(L_1) \lesssim N^2 \beta_1/\beta_0 \tag{5.7}$$

and

$$\mathrm{cond}(\tilde{Y}^{-1} L_1^{-3/2} \tilde{V}^{\mathrm{sym}}) \le \mathrm{cond}(\tilde{Y})\,\mathrm{cond}(L_1)^{3/2} \lesssim N^3 \beta_1/\beta_0. \tag{5.8}$$

Since these bounds are not uniform in N, the question arises of whether we can define a better scaling for the eigenvectors to improve them. Since $\tilde{\Lambda}$ is bounded independently of N, a uniform bound for the condition number of the matrix of eigenvectors $\tilde{Y}^{-1}L_1^{-1}\tilde{V}^{\mathrm{sym}}$ would imply a uniform bound on the condition number of $L_1^{-1/2}L_0^{\mathrm{qcf}}L_1^{-1/2}$. This, however, would contradict [6, Thm. 4.3], which states that $\mathrm{cond}(L_1^{-1/2}L_0^{\mathrm{qcf}}L_1^{-1/2}) \gtrsim N^{1/2}$, and hence no choice of eigenbasis can achieve an upper bound in (5.7) that is uniform in N.

5.1.4. Convergence rates for P-GMRES. From the foregoing discussion we obtain the following convergence rates for the P-GMRES solution of (5.1) (see [8, sects. 6.2 and 6.3] for details of these derivations):

For the standard left-preconditioned GMRES algorithm, we obtain bounds on the preconditioned residual (5.2),

$$\|L_1^{-1}r^{(m)}\| \le CN^3q^m\|L_1^{-1}r^{(0)}\|, \tag{5.9}$$

where $C > 0$ and $q \in (0,1)$ are independent of N and $\mathcal{A}$.

For the left-preconditioned P-GMRES algorithm, which minimizes the preconditioned residual in the norm induced by L_1, we obtain

$$\|L_1^{-1/2}r^{(m)}\| \le CN^2q^m\|L_1^{-1/2}r^{(0)}\|, \tag{5.10}$$

where $C \ge 0$ and $q \in (0,1)$ are independent of N and $\mathcal{A}$.

We also note that a finer analysis (see [8, sects. 6.2 and 6.3]) shows that both variants of P-GMRES reduce the residual to zero in at most $O(\#\mathcal{A})$ iterations.

5.2. Stability of L_0^{qcf} in $\mathcal{U}^{2,2}$. We define the discrete Sobolev-type norm

$$\|u\|_2 = \|Lu\| \qquad \text{for } u \in \mathbb{R}^N,$$

which is a norm on the space $\mathcal{U}$ of mean-zero functions, and denote the space $\mathcal{U}$ equipped with $\|\cdot\|_2$ by $\mathcal{U}^{2,2}$. Moreover, we denote the space $\mathcal{U}$ equipped with the norm $\|\cdot\| =: \|\cdot\|_0$ by $\mathcal{U}^{0,2}$. We are interested in the question of whether $L_0^{\mathrm{qcf}} : \mathcal{U}^{2,2} \to \mathcal{U}^{0,2}$ is stable, uniformly in N and $\mathcal{A}$.

To begin with, we note that

$$\|(L_0^{\mathrm{qcf}})^{-1}\|^{-1}_{L(\mathcal{U}^{0,2},\mathcal{U}^{2,2})} = \inf_{u\in\mathcal{U}\setminus\{0\}} \frac{\|L_0^{\mathrm{qcf}}u\|_0}{\|Lu\|_0} = \inf_{f\in\mathcal{U}\setminus\{0\}} \frac{\|L_0^{\mathrm{qcf}}L_1^{-1}f\|_0}{\|f\|_0};$$

thus, the question reduces to the analysis of the operator $L_0^{\mathrm{qcf}}L_1^{-1}$. Using the representation

$$\begin{aligned} L_0^{\mathrm{qcf}} &= L^{\mathrm{c}} + P_{\mathcal{U}}X(L^{\mathrm{a}} - L^{\mathrm{c}}) \\ &= W_F''L + P_{\mathcal{U}}X(L^{\mathrm{a}} - W_F''L), \\ &= W_F''[I + P_{\mathcal{U}}X(\tfrac{1}{W_F''}L^{\mathrm{a}}L_1^{-1} - I)]L, \end{aligned}$$

we obtain

$$L_0^{\mathrm{qcf}}L_1^{-1} = W_F''[I + P_{\mathcal{U}}X(\tfrac{1}{W_F''}L^{\mathrm{a}}L_1^{-1} - I)].$$

Application of Lemma 4.6 with $B = (\frac{1}{W_F''}L^{\mathrm{a}}L_1^{-1} - I)$ shows that it is invertible and provides uniform bounds on the inverse. Restricting the argument back to $\mathcal{U}$ we obtain the following theorem.

THEOREM 5.1. *Suppose that $W_F'' > 0$ and $L^{\rm a} \geq \gamma_{\rm a} L$; then $L_0^{\rm qcf}$ is invertible on $\mathcal{U}$ and $\|(L_0^{\rm qcf})^{-1}\|_{L(\mathcal{U}^{0,2},\mathcal{U}^{2,2})}$ is bounded above by a constant that depends only on W_F'', $\gamma_{\rm a}$, and $\|L^{\rm a} L_1^{-1}\|$. In particular, if (4.1) holds, then $\gamma_{\rm a} \geq W_F''$ and $\|(L_0^{\rm qcf})^{-1}\|_{L(\mathcal{U}^{0,2},\mathcal{U}^{2,2})}$ is bounded above by a constant that depends only on the coefficients ϕ_{rF}'', $r = 1, \ldots, R$, but is independent of N and $\mathcal{A}$.*

6. Conclusion. We have established a comprehensive ℓ^2-theory of a linearized force-based quasicontinuum (QCF) operator in one dimension. We have given elementary derivations in the case of second-neighbor interactions but have also provided proofs for arbitrary finite-range interactions. As immediate corollaries of our analysis we have also obtained new results on the convergence of (preconditioned) GMRES iterations and a new stability estimate in the space $\mathcal{U}^{2,2}$.

Our results rely heavily on the fact that the nonlinear QCF operator is linearized at a homogeneous deformation, and a question of immediate relevance is whether our results can be generalized, at least partially, to linearizations around nonuniform states. Even in small neighborhoods of homogeneous deformations it is unclear whether this can be done.

Second, we have relied heavily on the uniformity of the grid; however, in typical applications one would use a strongly graded mesh. We believe that, by applying the finite element theory for eigenvalue problems, our results partially generalize to the discretized case. We stress, however, that this would require a range of new results, in particular on the regularity of the QCF eigenfunctions.

Third, a generalization to two or three dimensions would have immense consequences, as no approach to the analysis of QCF in two or three dimensions exists at this point.

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